Comparing the molecular graph degeneracy of Wiener, Harary, Balaban, Randić and ZEP topological indices

ZOIŢA-MĂRIOARA BERINDE

ABSTRACT.

The aim of this paper is to show that the ZEP topological index has better discrimination power than four well known topological indices in molecular chemistry: Balaban index, Harary index, Randić index, and Wiener index.

REFERENCES

[1] Balaban, A. T., *Applications of graph theory in chemistry*, J. Chem. Inf. Comput. Sci., **25** (1985), 334–343
[2] Balaban, A. T., *Can topological indices transmit information on properties but not on structure?*, J. Comput. Aided Design, **19** (2005), 651–660
[3] Barysz, M., Jashari, G., Lall, R. S., Srivastaya, V. K. and Trinajstić, N., On the Distance Matrix of Molecules Containing Heteroatoms, in *Chemical Applications of Graph Theory and Topology*, King, R. B. (Ed), Elsevier, Amsterdam, 1983, 222–230
[4] Berinde, Z., *Applications of Molecular Topology in the Study of Physico-chemical Properties of Organic Compounds* (in Romanian), Cub Press 22, Baia Mare, 2001
[5] Berinde, Z., *Consideraţii privind modelarea matricială a compuşilor halogenaţi*, Rev. Chim. (Bucureşti), **52** (2001), No. 12, 788–792
[6] Berinde, Z., *Un nou indice topologic de tip Randić*, Rev. Chim. (Bucureşti), **53** (2002), No. 1, 812–816
[7] Berinde, Z. and Drinkal, C., *On a local invariant for modeling molecular double bonds graphs*, Chem. Bull. "Politehnica" Univ. (Timişoara), **49 (63)** (2004), No. 1-2, 8–10
[8] Berinde Z. and Drinkal, C., *Molecular modelling of molar refraction for alkanes*, Chem. Bull. "Politehnica" Univ. (Timişoara), **49 (63)** (2004), No. 1-2, 4–7
[9] Berinde, Z., *Vertex- and edge-weighted molecular graphs for amines*, Rev. Roum. Chim., **51** (2006), No. 11, 1131–1135
[10] Berinde, Z., *QSPR modelling of molar volume of alkanes using the ZEP topological index*, Creat. Math. Inform. **17** (2008), No. 3, 308–312
[11] Berinde, Z., *Matrix mathematical models used in the representation of molecular structures*, Sc. Stud. Res. Ser. Math. Inf., **19** (2009), No. 2, 59–70
[12] Berinde, Z., *A QSPR study of hydrophobicity of phenols and 2-(aryloxy-α-acetyl)-phenoxathiin derivatives using the topological index ZEP*, Creat. Math. Inform., **22** (2013), No. 1, 33–40
[13] Diudea M. and Ivanciuc, O., *Molecular Topology* (in Romanian), Comprex, Cluj-Napoca, 1995
[14] Estrada, E., *Edge adjacency relationships in molecular graphs containing heteroatoms: A novel topological index related to molar volume*, J. Chem. Inf. Comput. Sci., **35** (1995), 701–707
[15] Faulon, J.-L., Brown, W. M., and Martin, S., *Reverse engineering chemical structures from molecular descriptors: how many solutions?*, J. Comput. Aided Design, **19** (2005), 637–650
[16] Ivanciuc, O., Balaban, T.-S., and Balaban, A., *Chemical graphs with degenerate topological indices based on information on distances*, J. Math. Chem., **14** (1993), 21–33
[17] Nikolić, S., Plavšić, D. and Trinastić, N., *On the Balaban-like topological indices*, MATHCH, **44** (2001), 361–386
[18] Plavšić, D., Nikolić, S. and Trinastić, N., *On the Harary index for the characterisation of chemical graphs*, J. Math. Chem., **12** (1993), 235–250
[19] Randić, M., *On characterization of molecular branching*, J. Amer. Chem. Soc., **97** (1975), 6609–6615
[20] Randić, M., *Novel Graph Theoretical Approach to Heteroatoms in Quantitative Structure-Activity Relationships*, Chemometrics Intel. Lab. Syst., **10** (1991), 213–227
[21] N. Trinajstić, *Chemical Graph Theory* , 2nd revised edition, vol. II, CRC Press, Boca Raton, Florida, 1992
[22] Wiener, H., *Structural determination of paraffins boiling points*, J. Amer. Chem. Soc., **69** (1947), 17–20
[23] Dragon Evaluation for Windows (Software for Molecular Descriptors calculations), Version 5.4, 2006, Talete srl, http://www.talete.mi.it/
[24] Molecular Modeling Pro, Version 6.10 trial, www.norgwyn.com/

DEPARTMENT OF CHEMISTRY AND BIOLOGY
NORTH UNIVERSITY CENTER AT BAIA MARE
TECHNICAL UNIVERSITY OF CLUJ-NAPOCA
VICTORIEI 76, 430122 BAIA MARE, ROMANIA
E-mail address: zoitaberinde@ubm.ro
E-mail address: zoita_berinde@yahoo.com